

Time Evolution of States for Open Quantum Systems. The quadratic case

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Abstract

Our main goal in this paper is to extend to any system of coupled quadratic Hamiltonians some properties known for systems of quantum harmonic oscillators related with the Brownian Quantum Motion model. In a first part we get a rather general formula for the purity (or the linear entropy) in a short time approximation. In a second part we establish a master equation (or a Fokker-Planck type equation) for the time evolution of the reduced matrix density for bilinearly coupled quadratic Hamiltonians. The Hamiltonians and the bilinear coupling can be time dependent.

Moreover we give an explicit formula for the solution of this master equation so that the time evolution of the reduced density at time t is connected with the reduced density at initial time t_0 for $t_0 \leq t < t_0 + t_c$ where $t_c \in]0, \infty]$ is a critical time but reversibility is lost for $t \geq t_0 + t_c$.

1 Introduction

The general setting considered here is a quantum system (S) interacting with an environment (E) . The total system $(S) \cup (E)$ is supposed to be an isolated quantum system and we are interested in dynamical properties of (S) alone, which is an open system because of its interactions with (E) . In particular during the time evolution the energy of (S) is not preserved and its evolution is not determined by a Schrödinger or Liouville-von Neumann equation unlike for the total system $(S) \cup (E)$.

The Hilbert space of the total system $(S) \cup (E)$ is the tensor product $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$ ¹ and its Hamiltonian \hat{H} is decomposed as follows:

$$\hat{H} = \underbrace{\hat{H}_S \otimes \mathbb{I} + \mathbb{I} \otimes \hat{H}_E}_{\hat{H}_0} + \hat{H}_I = \hat{H}_0 + \hat{V} \quad (1.1)$$

$(S) \cup (E)$ is isolated by assumption and its evolution obeys the Schrödinger (or Liouville-von Neumann) equation with the Hamiltonian \hat{H} .

All Hamiltonians here are self -adjoint operators on their natural domain, \hat{H} and $\hat{H}_I = \hat{V}$ are defined in \mathcal{H} , \hat{H}_S in \mathcal{H}_S , \hat{H}_E in \mathcal{H}_E . Moreover most of the results stated here are valid when the Hamiltonians are time dependent, assuming that their propagators exist as unitary operators in the corresponding Hilbert space.

Quantum observables are denoted with a hat accent, the corresponding classical observables (also named Wigner function or Weyl-symbols) are written by erasing the hat.

We don't give here more details concerning the domains, these will be clear in the applications.

We assume that the interacting potential \hat{V} has the following form

$$\hat{V} = \sum_{1 \leq j \leq m} \hat{S}_j \otimes \hat{E}_j \quad (1.2)$$

where \hat{S}_j and \hat{E}_j are self-adjoint operators in \mathcal{H}_S , \mathcal{H}_E respectively.

¹ when the spaces are infinite dimensional we mean here that $\mathcal{H}_S \otimes \mathcal{H}_E$ is the Hilbert tensor product, completion of the algebraic tensor product

Recall that a density matrix $\hat{\rho}$ is a positive class trace operator with trace one ($\text{tr}\hat{\rho} = 1$). $\hat{\rho}$ is a state of the total system $(S) \cup (E)$ in the Hilbert space \mathcal{H} . The time evolution of $\hat{\rho}$ obeys the following Liouville-von Neumann equation:

$$\dot{\hat{\rho}} = i^{-1}[\hat{H}, \hat{\rho}], \quad \hat{\rho} : t \mapsto \hat{\rho}(t) \quad (1.3)$$

Time derivatives are denoted by a dot, $[\cdot, \cdot]$ denotes the commutator of two observables.

We assume that for $t = 0$ the system and the environment are decoupled :

$$\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0), \quad \hat{\rho}_{S,E}(0) \text{ are density matrices in } \mathcal{H}_{S,E} \quad (1.4)$$

and the state $\hat{\rho}_S(0)$ of the system is pure i.e is an orthogonal projector on a unit vector ψ of \mathcal{H}_S . A non pure state will be called a mixed state. A density matrix $\hat{\rho}_S$ is a mixed state if and only if $\hat{\rho}_S$ has an eigenvalue λ , such that $0 < \lambda < 1$.

Si, if $\hat{\rho}$ is a pure state then $\hat{\rho} = \Pi_\psi$, $\psi \in \mathcal{H}$, $\|\psi\| = 1$ where $\Pi_\psi(\eta) = \langle \psi, \eta \rangle \psi$.

The general problem for open systems is to describe the evolution $\hat{\rho}_S(t)$ of the density matrix of the system (S) . In particular an important physical question is: when the state $\hat{\rho}_S(t)$ is pure or mixed? To decide if a state is pure or not we consider the purity function

$$p_{ur}(t) = \text{tr}_S(\hat{\rho}_S(t)^2)$$

The function $S_\ell(t) = 1 - p_{ur}(t)$ is called the linear entropy. The Boltzman-von Neumann entropy is $S_{BN} = -\text{tr}_S(\hat{\rho}_S \log \hat{\rho}_S)$.

We clearly have $0 \leq p_{ur}(t) \leq 1$. It is not difficult to see that $\rho_S(t)$ is pure if and only if $p_{ur}(t) = 1$.

With our assumption, 0 is a maximum for p_{ur} so we have $\ddot{p}_{ur}(0) \leq 0$ and if $\ddot{p}_{ur}(0) < 0$ then for $0 < t < \varepsilon$, $\hat{\rho}_S(t)$ is a mixed state for ε small enough.

For isolated (closed) systems, if the initial state is pure then it stays pure at every time, as it can be easily seen using equation (1.3).

So our first step in this paper is to compute $\ddot{p}_{ur}(0)$. In particular for a large class of models, including the Quantum Brownian Motion, we shall prove that $\ddot{p}_{ur}(0) < 0$ so for these models the state of the system becomes very quickly decoherent and entangled with the environment.

Our second goal is to compute the time evolution $\hat{\rho}_S(t)$ of the state of the system. We know that $\hat{\rho}_S(t)$ does not satisfy a Liouville- von Neumann equation because the system is open.

We shall prove that for any time dependent quadratic systems, $\hat{\rho}_S(t)$ obeys an exact "master equation" similar to a Fokker-Planck type equation, with time dependent coefficients, and from this equation we can get an explicit formula for $\hat{\rho}_S(t)$.

This could be a first step for more general systems in the semi-classical régime .

Let us recall a mathematical definition for $\rho_S(t)$ and related properties and notations.

This can be done by introducing partial trace (or relative trace) over the environment for a state $\hat{\rho}$ of the global system.

Definition 1.1 Let \hat{A} be a class-trace operator in $\mathcal{H}_S \otimes \mathcal{H}_E$. We denote $\text{tr}_E \hat{A}$ the unique trace-class operator on \mathcal{H}_S satisfying, for every bounded operator \hat{B} on \mathcal{H}_S ,

$$\text{tr}_S \left((\text{tr}_E \hat{A}) \hat{B} \right) = \text{tr} \left(\hat{A} (\hat{B} \otimes \mathbb{I}_E) \right) \quad (1.5)$$

We have denoted "tr" the trace in the total space \mathcal{H} , $\text{tr}_{S,E}$ the trace in $\mathcal{H}_{S,E}$ respectively.

Of course we have $\text{tr}(\hat{B} \otimes \hat{C}) = \hat{B} \cdot (\text{tr}_E \hat{C})$ if \hat{B} and \hat{C} are trace class operators in \mathcal{H}_S and \mathcal{H}_E respectively.

If $\hat{\rho}$ is a density matrix in \mathcal{H} then $\text{tr}_E \hat{\rho}$ is a density matrix in \mathcal{H}_S , called the reduced density matrix or the reduced state.

From (1.5) we can compute the matrix element of $\text{tr}_E \hat{A}$ by the formula

$$\langle \psi, (\text{tr}_E \hat{A}) \varphi \rangle = \text{tr} \left(\hat{A} (\Pi_{\psi, \varphi} \otimes \mathbb{I}_E) \right), \quad \forall \psi, \varphi \in \mathcal{H}_S.$$

The partial trace was introduced in quantum mechanics to explain quantum phenomena like *entanglement* and *decoherence* (see [18, 19] for more details).

Let $\Psi \in \mathcal{H}_S \otimes \mathcal{H}_E$, $\Psi = \sum_{1 \leq j \leq N} \psi_j \otimes \eta_j$. Ψ is a pure state in $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. Let us compute the partial trace of Π_Ψ in \mathcal{H}_E . Applying Definition 1.1 we easily get

$$\text{tr}_E(\Pi_\Psi) = \sum_{1 \leq j, k \leq N} \langle \eta_j, \eta_k \rangle \Pi_{\psi_j, \psi_k} \quad (1.6)$$

where Π_{ψ_j, ψ_k} is the rank one operator in \mathcal{H}_S : $\Pi_{\psi_j, \psi_k}(\varphi) = \langle \psi_j, \varphi \rangle \psi_k$.

Decoherence means in particular that there exists a basis $\{\eta_j\}$ such that $|\langle \eta_j, \eta_k \rangle|$ becomes very small for $j \neq k$, so that $\text{tr}_E(\Pi_\Psi)$ is very close to $\sum_{1 \leq j \leq N} \Pi_{\psi_j}$ hence quantum interferences for the system (S) are lost.

Formula (1.5) is an operator version of Fubini integration theorem as we can see in the Weyl quantization setting.

Let $\mathcal{H}_S = L^2(\mathbb{R}^d)$, $\mathcal{H}_E = L^2(\mathbb{R}^N)$. Denote $z = (x, \xi) \in \mathbb{R}^{2d}$, $u = (y, \eta) \in \mathbb{R}^{2N}$, $A = \sigma_w \hat{A}$ the Weyl symbol of \hat{A} in the Schwartz space $\mathcal{S}(\mathbb{R}^{2(d+N)})$ (see [6] for more details) then the Weyl symbol of $\text{tr}_E \hat{A}$ is

$$\sigma_w(\text{tr}_E \hat{A})(z) = (2\pi)^{-N} \int_{\mathbb{R}^{2N}} A(z, u) du. \quad (1.7)$$

Our main applications here concerns the Weyl-quadratic case where :

- H_S, H_E are quadratic Hamiltonians (generalized harmonic oscillators) respectively in the phase spaces $\mathbb{R}^{2d}, \mathbb{R}^{2N}$.
- \hat{H}_S, \hat{H}_E are quantum Hamiltonians (Weyl quantization of H_S respectively H_E) in $L^2(\mathbb{R}^d)$ respectively $L^2(\mathbb{R}^N)$.
- $\hat{\rho}_S$ is the projector on $\psi \in \mathcal{S}(\mathbb{R}^d)$.
- ρ_E is a Gaussian with 0 means.
- S_j resp. E_j are linear forms on \mathbb{R}^{2d} resp. \mathbb{R}^{2N} (bilinear coupling).

In applications one consider thermal equilibrium states for environment: $\hat{\rho}_E = Z(\beta)^{-1} e^{-\beta \hat{K}_E}$ where K_E is a quadratic form, positive-definite and $\beta = \frac{1}{T}$, $T > 0$ is the temperature, $Z(\beta) = \text{tr}(e^{-\beta \hat{K}_E})$.

In this setting it is possible to find the exact time dependent master equation satisfied by $\hat{\rho}_S(t)$, as we shall see in the second part of this paper ($\hat{\rho}_E$ can be any environment state) and to solve this equation when the classical dynamics of the total system $(S) \cup (E)$ is known.

Let us remark that there exists a general formula, called Kraus formula, giving the time evolution of the reduced system: $\hat{\rho}_S(t) = \text{tr}_E(U(t)\hat{\rho}(0)U^*(t))$ where $\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0)$ and $U(t) = e^{-it\hat{H}}$ (see [19, 3]):

$$\hat{\rho}_S(t) = \sum_{j, \ell} \hat{K}_{j, \ell}(t) \hat{\rho}_S(0) \hat{K}_{j, \ell}(t)^* \quad (1.8)$$

where the Kraus operators $\hat{K}_{j, \ell}(t)$ depends on $\hat{\rho}_E(0)$ and $U(t)$. But the operators $\hat{K}_{j, \ell}(t)$ are not explicitly known, so formula (1.8) is not easy to use to get properties of $\hat{\rho}_S(t)$.

2 A general computation

It is easier here to consider the interaction formulation of quantum mechanics to "eliminate" the "free" (non-interacting) evolution: $U_0(t) = e^{-it\hat{H}_0}$. In this section we consider the general setting described in the introduction. No restrictions are necessary for the Hamiltonians \hat{H}_S, \hat{H}_E , we only need that

the interaction Hamiltonian has the shape (1.2). As it is well known the time evolution (1.3) is given by the Schrödinger evolution

$$\hat{\rho}(t) = U(t)\hat{\rho}(0)U(t)^*, \quad U(t) = e^{-it\hat{H}}.$$

For simplicity we assume here that all Hamiltonians are time independent but the results are also valid if H, S_j, E_j are time dependent. In this case we have $U(t) = U(t, 0)$ where 0 is the initial time. Introduce the inter-acting evolution

$$\hat{\rho}^{(I)}(t) = U_0(t)^*\hat{\rho}(t)U_0(t),$$

(1.3) becomes

$$\dot{\hat{\rho}}^{(I)} = i^{-1}[V(t), \hat{\rho}^{(I)}], \quad (2.9)$$

where

$$\hat{V}(t) = U_0(t)^*\hat{V}U_0(t) = \sum_{1 \leq j \leq m} S_j(t) \otimes E_j(t),$$

with $\hat{S}_j(t) = e^{it\hat{H}_S}\hat{S}_j e^{-it\hat{H}_S}$ and $\hat{E}_j(t) = e^{itH_E}\hat{E}_j e^{-itH_E}$. The useful fact here is that the shape of the interaction $\hat{V}(t)$ is the same for all $t \in \mathbb{R}$ (1.2). Let us remark again that technical assumptions are necessary for rigorous statements.

We see easily that

$$\hat{\rho}_S^{(I)}(t) := \text{tr}_E(\hat{\rho}^{(I)}(t)) = e^{it\hat{H}_S}\hat{\rho}_S(t)e^{-it\hat{H}_S}.$$

We want to consider the purity $p_{ur}(t) = \text{tr}_S(\hat{\rho}_S^{(I)}(t)^2)$. We shall use now the simpler notation $\hat{r}(t) = \hat{\rho}_S^{(I)}(t)$.

Using cyclicity of the trace we have

$$\dot{p}_{ur}(t) = 2\text{tr}_S(\hat{r}(t)\dot{\hat{r}}(t)) \quad (2.10)$$

$$\ddot{p}_{ur}(t) = 2\left(\text{tr}_S(\hat{r}(t)\ddot{\hat{r}}(t)) + \text{tr}_S(\dot{\hat{r}}(t))^2\right) \quad (2.11)$$

We have, at time $t = 0$,

$$\dot{\hat{r}}(0) = i^{-1}\text{tr}_E[\hat{V}, \hat{\rho}_S \otimes \hat{\rho}_E], \quad (2.12)$$

$$\ddot{\hat{r}}(0) = i^{-1}\text{tr}_E[\dot{\hat{V}}, \hat{\rho}_S \otimes \hat{\rho}_E] - \text{tr}_E[\hat{V}, [\hat{V}, \hat{\rho}_S \otimes \hat{\rho}_E]]. \quad (2.13)$$

Lemma 2.1 *Assume that $\hat{\rho}_S(0)$ is a pure state and that $\text{tr}_E(\hat{\rho}_E(0)\hat{E}_j) = 0$ for every $1 \leq j \leq m$. Then we have*

$$\dot{\hat{r}}(0) = 0.$$

Proof. For simplicity we denote $\hat{\rho}_E = \hat{\rho}_E(0)$, $\hat{\rho}_S = \hat{\rho}_S(0)$. Using the splitting assumption on \hat{V} we have

$$[\hat{V}, \hat{\rho}_S \otimes \hat{\rho}_E] = \left[\sum_{1 \leq j \leq m} \hat{S}_j \otimes \hat{E}_j, \hat{\rho}_S \otimes \hat{\rho}_E \right] \quad (2.14)$$

$$= \sum_{1 \leq j \leq m} \hat{S}_j \hat{\rho}_S \otimes \hat{E}_j \hat{\rho}_E - \hat{\rho}_S \hat{S}_j \otimes \hat{\rho}_E \hat{E}_j \quad (2.15)$$

So taking the E -trace we have

$$\text{tr}_E([\hat{V}, \hat{\rho}_S \otimes \hat{\rho}_E]) = \sum_{1 \leq j \leq m} [\hat{S}_j, \hat{\rho}_S] \text{tr}_E(\hat{\rho}_E \hat{E}_j)$$

□

Lemma 2.2 *We have*

$$\mathrm{tr}_S \left(\mathrm{tr}_E [\dot{\hat{V}}, \hat{\rho}_S \otimes \hat{\rho}_E] \hat{\rho}_S \right) = 0 \quad (2.16)$$

Proof. This follows from the definition of the relative trace tr_E and cyclicity of the trace. We have

$$\mathrm{tr}_S \left(\mathrm{tr}_E [\dot{\hat{V}}, \hat{\rho}_S \otimes \hat{\rho}_E] \hat{\rho}_S \right) = \mathrm{tr} \left([\dot{\hat{V}}, \hat{\rho}_S \otimes \hat{\rho}_E] \hat{\rho}_S \otimes 1 \right)$$

This is 0 because $\hat{\rho}_S \otimes \hat{\rho}_E$ and $\hat{\rho}_S \otimes 1$ commute. \square

Finally, using the identity

$$[\hat{V}, [\hat{V}, \hat{\rho}]] = \hat{V}^2 \hat{\rho} + \hat{\rho} \hat{V}^2 - 2\hat{V} \hat{\rho} \hat{V}$$

with the same argument as in Lemma 2.1 we get the following proposition:

Proposition 2.3 *Under the condition of Lemma 2.1 we have*

$$\ddot{p}_{ur}(0) = -4\mathrm{tr} \left(\hat{V} \hat{\rho}(0) \hat{V} (\hat{\rho}_S^\perp \otimes \mathbb{I}) \right) \quad (2.17)$$

with $\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0)$ and $\hat{\rho}_S^\perp = \mathbb{I} - \hat{\rho}_S(0)$.

In particular if $(\hat{\rho}_S^\perp \otimes \mathbb{I}) \hat{V} \hat{\rho} \hat{V}$ is not 0 in the range of $\hat{\rho}_S^\perp \otimes \mathbb{I}$ then $\ddot{p}_{ur}(0) < 0$ and for any $t \neq 0$, t small enough, $\hat{\rho}_S(t)$ is a mixed state.

The formula (2.17) can be written in a more suggestive form, using the decomposition of \hat{V} to separate the contributions of the system and its environment. The result is

$$\ddot{p}_{ur}(0) = -4 \sum_{1 \leq j, j' \leq m} \left(\mathrm{tr}_S(\hat{\rho}_S \hat{S}_{j'} \hat{S}_j) - \mathrm{tr}_S(\hat{\rho}_S \hat{S}_{j'} \hat{\rho}_S \hat{S}_j) \right) \mathrm{tr}_E(\hat{\rho}_E \hat{E}_{j'} \hat{E}_j) \quad (2.18)$$

This formula has the following statistical interpretation, introducing the quantum covariance matrices:

$$\Gamma_{j',j}^{(S)} = \mathrm{tr}_S(\hat{\rho}_S \hat{S}_{j'} \hat{S}_j) - \mathrm{tr}_S(\hat{\rho}_S \hat{S}_{j'} \hat{\rho}_S \hat{S}_j), \quad \Gamma_{j',j}^{(E)} = \mathrm{tr}_E(\hat{\rho}_E \hat{E}_{j'} \hat{E}_j) \quad (2.19)$$

so we have

$$\ddot{p}_{ur}(0) = -4\mathrm{tr}_{\mathbb{R}^m}(\Gamma^{(S)}(\Gamma^{(E)})^\top). \quad (2.20)$$

Then we get a short time asymptotic expansion using Taylor formula

$$p_{ur}(t) = \frac{\ddot{p}_{ur}(0)}{2} t^2 + O(t^3), \quad t \searrow 0.$$

So if from formula (2.20) we can infer that $\ddot{p}_{ur}(0) < 0$ then we get that $\hat{\rho}_S(t)$ is a mixed state for $t > 0$ small enough.

3 Application to the quadratic case

We consider here the Weyl-quadratic case described in the introduction (all Hamiltonians are now supposed to be quadratic).

We use the following basic property of Weyl quantization in \mathbb{R}^d : If A, B are Weyl symbols such that B is in the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ and A is a polynomial (or like a polynomial) then we have

$$\mathrm{tr}_{L^2(\mathbb{R}^d)}(\hat{A}\hat{B}) = (2\pi)^{-d} \int_{\mathbb{R}^{2d}} A(z)B(z)dz.$$

Let us compute $\ddot{p}_{ur}(0)$ using formula (2.19) and the Weyl symbols.

Note that $2\pi^{-d}\rho_S(z)dz$ and $(2\pi)^{-N}\rho_E(u)du$ are probabilities laws denoted by $\pi_S(z)dz$ and $\pi_E(u)du$

respectively.

$\hat{\rho}_S = \hat{\rho}(0)$ is a projector on a state ψ_0 of \mathcal{H}_S so we can compute

$$\begin{aligned} \text{tr}_S(\hat{\rho}_S \hat{S}_{j'} \hat{\rho}_S \hat{S}_j) &= \langle \psi_0, \hat{S}_j \psi_0 \rangle \langle \psi_0, \hat{S}_{j'} \psi_0 \rangle \\ &= \left(\int_{\mathbb{R}^{2d}} \pi_S(z) S_j(z) dz \right) \left(\int_{\mathbb{R}^{2d}} \pi_S(z) S_{j'}(z) dz \right). \end{aligned} \quad (3.21)$$

Let us introduce the commutators

$$s_{j'j} = [\hat{S}_{j'}, \hat{S}_j], \quad e_{j'j} = [\hat{E}_{j'}, \hat{E}_j]$$

We have

$$\begin{aligned} \text{tr}_S(\hat{\rho}_S \hat{S}_{j'} \hat{S}_j) &= \int_{\mathbb{R}^{2d}} \pi_S(z) S_{j'}(z) S_j(z) dz + \frac{1}{2i} s_{j'j} \\ \text{tr}_E(\hat{\rho}_E \hat{E}_{j'} \hat{E}_j) &= \int_{\mathbb{R}^{2N}} \pi_E(u) E_{j'}(u) E_j(u) du + \frac{1}{2i} e_{j'j}. \end{aligned} \quad (3.22)$$

Then we get

$$\begin{aligned} \ddot{p}_{ur}(0) &= -4 \sum_{j,j'} \left(\int_{\mathbb{R}^{2d}} \pi_S(z) S_{j'}(z) S_j(z) dz \right. \\ &\quad \left. - \left(\int_{\mathbb{R}^{2d}} \pi_S(z) S_j(z) dz \right) \left(\int_{\mathbb{R}^{2d}} \pi_S(z) S_{j'}(z) dz \right) \right) + \sum_{j,j'} s_{j'j} e_{j'j}. \end{aligned} \quad (3.23)$$

Let us introduce the classical (symmetric) covariance matrices

$$\Sigma_{jj'}^{(S)} = \int_{\mathbb{R}^{2d}} \pi_S(z) S_{j'}(z) S_j(z) dz - \left(\int_{\mathbb{R}^{2d}} \pi_S(z) S_j(z) dz \right) \left(\int_{\mathbb{R}^{2d}} \pi_S(z) S_{j'}(z) dz \right)$$

and

$$\Sigma_{jj'}^{(E)} = \int_{\mathbb{R}^{2N}} \pi_E(u) E_{j'}(u) E_j(u) du.$$

So we get

$$\ddot{p}_{ur}(0) = -4 \text{tr}_{\mathbb{R}^{2m}}(\Sigma^{(S)} \Sigma^{(E)}) + \sum_{1 \leq j, j' \leq m} s_{j'j} e_{j'j}. \quad (3.24)$$

We remark that in formula (3.24) r.h.s the first term is classical and the second term is a quantum correction q_c which vanishes if the coupling between the system and its environment is only in position (or momentum) variables (as it is usually in the literature).

Assume now that $S_j(z) = z_j$ and $E_j(u) = \sum_{1 \leq \ell \leq 2N} G_{j,\ell} u_\ell$, where $1 \leq j \leq 2d$. $G_{j,\ell}$ is a $2d \times 2N$ matrix with real coefficients. With these notations we have for the quantum correction

$$q_c = \sum_{1 \leq j, j' \leq 2d} s_{j'j} e_{j'j} = \text{tr}_{\mathbb{R}^{2d}}(J_S G J_E G^\top) \quad (3.25)$$

where J_S, J_E are respectively the matrix of the canonical symplectic form in \mathbb{R}^{2d} and \mathbb{R}^{2N} : $\sigma_S(z, z') = z \cdot J_S z'$, $\sigma_E(u, u') = u \cdot J_E u'$ (the scalar products are denoted by a \cdot).

For the "classical part" we have

$$-4 \text{tr}_{\mathbb{R}^{2m}}(\Sigma^{(S)} \Sigma^{(E)}) = -4 \text{tr}(G^\top \text{Cov}_{\rho_S} G \text{Cov}_{\rho_E}) \quad (3.26)$$

where G^\top is the transposed of the matrix G .

So we have proved the formula:

$$\boxed{\ddot{p}_{ur}(0) = -4 \text{tr}_{\mathbb{R}^{2N}}(G^\top \text{Cov}_{\pi_S} G \text{Cov}_{\pi_E}) + \text{tr}_{\mathbb{R}^{2d}}(J_S G J_E G^\top)} \quad (3.27)$$

where Cov_π is the covariance matrix for the quasi-probability π (the Wigner function of a pure state ψ is non negative if and only if ψ is a Gaussian by the Hudson theorem [6])

In the physicist literature [5, 3, 10] the following example is often considered: a quantum oscillator system is coupled with a bath of oscillators in a thermal equilibrium by their position variables. This is known as the Quantum Brownian Motion model. So we choose $d = 1$, $\rho_E = \rho_{\tau,E}$,

$$V(z, u) = x \cdot \sum_{1 \leq j \leq N} c_j y_j.$$

c_1, \dots, c_N are real numbers, $z = (x, \xi) \in \mathbb{R}^2$, $u = (y, \eta) \in \mathbb{R}^{2N}$ and $\rho_E = \rho_{\tau,E}$ where

$$\rho_{\tau,E} = (2\tau)^N \exp \left(-\tau \sum_{1 \leq j \leq 2N} u_j^2 \right)$$

τ is related to the temperature T by the formula $\tau = \tanh(T^{-1})$ (taking the Boltzmann constant $k = 1$). So we have $0 < \tau < 1$.

With these parameters we get

$$\ddot{p}_{ur}(0) = -\frac{2}{\tau}(c_1^2 + \dots + c_N^2)\text{Cov}_{x,x}(\psi_0), \quad (3.28)$$

where $\text{Cov}_{x,x}(\psi_0) = \int_{\mathbb{R}} x^2 |\psi_0(x)|^2 dx - (\int_{\mathbb{R}} x |\psi_0(x)|^2 dx)^2$. If the oscillators of the bath have different temperatures T_1, \dots, T_N then the result is

$$\ddot{p}_{ur}(0) = -2\left(\frac{c_1^2}{\tau_1} + \dots + \frac{c_N^2}{\tau_N}\right)\text{Cov}_{x,x}(\psi_0)$$

where $\tau_j = \tanh(T_j^{-1})$.

A more general bilinear coupling is

$$V(x, \xi; y, \eta) = x \cdot \left(\sum_{1 \leq j \leq N} c_j y_j + \sum_{1 \leq j \leq N} c_{j+N} \eta_j \right) + \xi \cdot \left(\sum_{1 \leq j \leq N} d_j y_j + \sum_{1 \leq j \leq N} d_{j+N} \eta_j \right)$$

The quantum correction q_c is

$$q_c = 2(d_1 c_{N+1} + \dots + d_N c_{2N}) - 2(c_1 d_{N+1} + \dots + c_N d_{2N})$$

Assume for simplicity that $c_j = 0$ for $j \geq N+2$ and $d_j = 0$ for $j \geq 2$. Then we find after computations:

$$\begin{aligned} \ddot{p}_{ur}(0) &= -\frac{4}{\tau}(c_1^2 + \dots + c_N^2 + c_{N+1}^2)\text{var}(\psi_0) \\ &\quad + 2c_1 d_1 \text{Cov}_{x,\xi}(\psi_0) + d_1^2 \text{Cov}_{\xi,\xi}(\psi_0) + 2c_{N+1} d_1 \end{aligned} \quad (3.29)$$

So we see that new quantum corrections appear when the coupling mixes positions and momenta variables.

Remark 3.1 In formula (3.29) we can see that if $\text{Cov}_{x,\xi}(\psi_0) = 0$ then $\ddot{p}_{ur}(0)$ can decrease or increase with the coefficient d_1 compared to the case $d_1 = 0$.

Remark 3.2 In the above computations we have assumed that the Planck constant \hbar is one. We can rewrite formula (3.27) including \hbar in Weyl quantization and we find

$$\ddot{p}_{ur}(0) = -4\hbar^{-2} \text{tr}_{\mathbb{R}^{2N}}(G^\top \text{Cov}_{\pi_S} G \text{Cov}_{\pi_E}) + \text{tr}_{\mathbb{R}^{2d}} J_S G J_E G^\top \quad (3.30)$$

As it is expected the "decoherence time" becomes very small when $\hbar \rightarrow 0$. The quantum correction has a meaning only when \hbar is not too small.

Remark 3.3 The environment state $\hat{\rho}_{\tau,E}$ is non-negative if and only $\tau \leq 1$. It is enough to prove that for $N = 1$. By an holomorphic extension argument in τ we can see that $\hat{\rho}_{\tau,E}$ is negative on the subspace of $L^2(\mathbb{R})$ spanned by the odd Hermite functions ψ_{2k+1} where $(-\frac{d^2}{dx^2} + x^2)\psi_k = (2k+1)\psi_k$. Let us prove this. Denote $\beta = \beta(\tau) = \arg \tanh(\tau)$, and $\hat{H}_{\text{osc}} = \frac{1}{2} \left(-\frac{d^2}{dx^2} + x^2 \right)$.

By the Mehler formula the Weyl symbol of $e^{-\beta \hat{H}_{\text{osc}}}$ is

$$\frac{1}{\cosh(\beta/2)} e^{-(\tanh(\beta/2)(x^2 + \xi^2))}$$

The thermal state at temperature $T = \frac{1}{\beta}$ is defined as

$$\hat{\mathcal{T}}_\beta = \frac{e^{-\beta \hat{H}_{\text{osc}}}}{\text{tr}(e^{-\beta \hat{H}_{\text{osc}}})}.$$

Its Weyl symbol is

$$\mathcal{T}_\beta(x, \xi) = \frac{1}{2} \tanh(\beta/2) e^{-\tanh(\beta/2)(x^2 + \xi^2)}.$$

Let us denote $W_k(x, \xi)$ the Wigner function of ψ_k . So we have

$$\langle \psi_k, e^{-\beta \hat{H}_{\text{osc}}} \psi_k \rangle = \frac{1}{\cosh(\beta)} \int_{\mathbb{R}^2} e^{-\tanh(\beta)(x^2 + \xi^2)} W_k(x, \xi) dx d\xi = e^{k+1/2}\beta \quad (3.31)$$

Using an holomorphic extension in the variable τ , for $\tau > 1$, we have

$$\beta(\tau) = \log \left(\frac{\tau + 1}{\tau - 1} \right) + \frac{i\pi}{2}$$

Hence we get

$$\langle \psi_k, \hat{\rho}_{\tau,E} \psi_k \rangle = \frac{(-1)^k (\tau - 1)^k}{2\pi(\tau + 1)^{k+1}}, \quad \forall \tau > 1. \quad (3.32)$$

So if $\tau > 1$ $\hat{\rho}_{\tau,E}$ is negative on ψ_k for k odd. \square

We can apply these results to give a simple proof that the state the system (S) is corollated with the environment (E) for any $t > 0$ small enough. Here we assume that both $\hat{\rho}_S(0)$ and $\hat{\rho}_E(0)$ are Gaussian pure states. A more general result will be given in Proposition 4.15.

Corollary 3.4 Let $\hat{\rho}(t) = U(t) (\hat{\rho}_S(0) \otimes \hat{\rho}_E(0)) U^*(t)$ be the time evolution of $(S) \cup (E)$. Assume that $\ddot{p}_{ur}(0) \neq 0$ (see formula (3.27)). Then there exists $\varepsilon > 0$ such that for every $t \in]0, \varepsilon]$ we have

$$\hat{\rho}(t) \neq \hat{\rho}_S(t) \otimes \hat{\rho}_E(t). \quad (3.33)$$

Proof. We shall prove (3.33) by contradiction. Assume that there exists a sequence of times $t_n > 0$, $\lim_{n \rightarrow +\infty} t_n = 0$ such that

$$\hat{\rho}(t_n) = \hat{\rho}_S(t_n) \otimes \hat{\rho}_E(t_n).$$

Let us remark that if such a decomposition exists then necessarily we have $\hat{\rho}_S(t_n) = \text{tr}_E(\hat{\rho}(t_n))$ and $\hat{\rho}_E(t_n) = \text{tr}_S(\hat{\rho}(t_n))$.

For $t = t_n$ we have

$$\text{tr}(\hat{\rho}(t)^2) = \text{tr}_S(\hat{\rho}_S(t)^2) \text{tr}_E(\hat{\rho}_E(t)^2)$$

From the above result applied to (S) and (E) we have

$$\text{tr}(\hat{\rho}(t)^2) = (1 - c_S t^2 + O(t^3))(1 - c_E t^2 + O(t^3)) = 1 - (c_S + c_E)t^2 + O(t^3)$$

where all the constants c_S, c_E are positive. So we get a contradiction because $\text{tr}(\hat{\rho}(t)^2) = \text{tr}(\hat{\rho}(0)^2)$ is independent on t . \square

In [8] the authors proved for the quantum Brownian motion that is possible to find a Gaussian initial state of the system and a temperature T of the environment such that $\hat{\rho}(t)$ is not entangled for all times in $[0, +\infty[$.

4 The master equation in the Weyl-quadratic case

4.1 General quadratic Hamiltonians

In this section we find a time dependent partial differential equation (often called the master equation) satisfied by the reduced density matrix $\hat{\rho}_S$ of the open system (S). Moreover this equation can be solved explicitly using the well known characteristics method.

We extend here to any quadratic Hamiltonians with arbitrary bilinear coupling, several results proved in many places [16, 14, 13, 10] for the quantum Brownian motion model with bilinear position coupling. Our results are inspired by the paper [10] but do not use the path integral methods as in the papers quoted above. Another difference is that in our case the number N of degrees of freedom for the environment is fixed and finite and the number d of degree of freedom for the system is also finite and arbitrary.

There exist many papers in the physicist literature concerning exact or approximated master equation for the quantum Brownian motion model (see the Introduction and References in [10]).

Here we assume that H_S and H_E are quadratic Weyl symbols of \hat{H}_S and \hat{H}_E respectively. We denote Φ_0^t the Hamiltonian flow generated by H_0 and Φ^t the Hamilton flow generated by $H = H_0 + V$. V is a bilinear coupling between the system and the environment : $V(z, u) = z \cdot G u$ where G is a linear map from \mathbb{R}^{2N} in \mathbb{R}^{2d} (note that the coupling can mix positions and momenta variables).

Recall that \mathbb{R}^{2d} (resp. \mathbb{R}^{2N}) is the classical phase space of the system (resp. the environment). $\Psi^t = \Phi_0^{-t} \Phi^t$ is the interacting flow in the global phase space $\mathbb{R}^{2(d+N)}$. The phase space of the global system is identified to the direct sum $\mathbb{R}^{2d} \oplus \mathbb{R}^{2N}$ and in this decomposition the flows are represented by 4 matrix blocks.

$$\Psi^t = \begin{pmatrix} \Psi_{ii}^t & \Psi_{ie}^t \\ \Psi_{ei}^t & \Psi_{ee}^t \end{pmatrix}$$

The "free" evolution is diagonal

$$\Psi_0^t = \begin{pmatrix} \Phi_S^t & 0 \\ 0 & \Phi_E^t \end{pmatrix}$$

and the interacting classical Hamiltonian is

$$H_I(t, z, u) = V(t, z, u) = z \cdot G(t)u, \text{ where } G(t) = (\Phi_S^t)^\top \cdot G \cdot \Phi_E^t.$$

The classical interacting evolution is given by the equation

$$\dot{\Psi}^t = J \nabla_{z,u}^2 V(t) \Psi^t, \text{ with } J = \begin{pmatrix} J_S & 0 \\ 0 & J_E \end{pmatrix},$$

where $\nabla_{z,u}^2 V(t)$ is the Hessian matrix in variables $(z, u) \in \mathbb{R}^{2d} \times \mathbb{R}^{2N}$.

So for the block components of the interacting dynamics we have

$$\dot{\Psi}_{ii}^t = J_S G(t) \Psi_{ei}^t, \quad \dot{\Psi}_{ie}^t = J_S G(t) \Psi_{ee}^t \quad (4.34)$$

$$\dot{\Psi}_{ei}^t = J_E G(t)^\top \Psi_{ii}^t, \quad \dot{\Psi}_{ee}^t = J_E G(t)^\top \Psi_{ie}^t. \quad (4.35)$$

Because all the Hamiltonians considered here are quadratic (eventually time dependent) they generate well defined quantum dynamics in Hilbert spaces $L^2(\mathbb{R}^n)$ where $n = d$ (system (S)), $n = N$ (environment (E)) and $n = d + N$ (global system ($S \cup E$)).

Recall the notations $U(t) = e^{-it\hat{H}}$, $U_0(t) = e^{-it\hat{H}_0}$, $U_S(t) = e^{-it\hat{H}_S}$, $U_E(t) = e^{-it\hat{H}_E}$. We have $U_0(t) = U_S(t) \otimes U_E(t)$ and the quantum interacting dynamics $U_I(t) = U_0(t)^* U(t)$.

At time $t = 0$ we assume that $\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0)$ where $\hat{\rho}_S$ (resp. $\hat{\rho}_E$) is a density matrix in the Hilbert space $\mathcal{H}_S = L^2(\mathbb{R}^d)$ (resp. in $\mathcal{H}_E = L^2(\mathbb{R}^N)$).

ρ , ρ_S , ρ_E are the Weyl symbols (i.e the Weyl-Wigner functions, with $\hbar = 1$, of the corresponding density matrices).

The coefficients of the quadratic forms H_S, H_E, V may be time dependent. In this case $U(t)$ means $U(t, 0)$ where $U(t, s)$ is the propagator solving

$$i \frac{\partial}{\partial t} U(t, s) = \hat{H} U(t, s), \quad U(s, s) = \mathbb{I}_{\mathcal{H}}.$$

It is well known that for quadratic Hamiltonians, every mixed state $\hat{\rho}$ of $(S) \cup (E)$ propagates according the classical evolution (see [6] for details)

$$\hat{\rho}(t) := U(t) \hat{\rho}(0) U(t)^*, \quad \rho(t, X) = \rho(0, \Phi^{-t} X), \quad X \in \mathbb{R}^{2(d+N)} \quad (4.36)$$

Our aim is to compute $\hat{\rho}_S(t) = \text{tr}_E(\hat{\rho}(t))$. The Weyl symbol of $\hat{\rho}_S(t)$ is given by the following integral

$$\rho_S(t, z) = \int_{\mathbb{R}^{2N}} \rho(t, z, u) du \quad (4.37)$$

In particular if $\rho(0)$ is Gaussian in all the variables $X = (z, u) \in \mathbb{R}^{2d} \times \mathbb{R}^{2N}$ then $\rho_S(t, z)$ is Gaussian in z . Nevertheless a direct computation on the formula (4.37) seems not easy to perform, so a different strategy will be used.

4.2 Gaussian mixed states

Let us consider a very useful class of matrix densities with Gaussian symbols; they are called Gaussian mixed states. For the reader convenience we recall here some well known results.

Definition 4.1 *A density matrix $\hat{\rho}$ in the Hilbert space $L^2(\mathbb{R}^n)$ is said Gaussian if its Weyl symbol ρ is a Gaussian $\rho^{\Gamma, m}$ where Γ is the covariance matrix (positive-definite $2n \times 2n$ matrix) and $m \in \mathbb{R}^{2d}$ the mean of ρ . So we have*

$$\rho^{\Gamma, m}(z) = c_{\Gamma} e^{-\frac{1}{2}(z-m) \cdot \Gamma^{-1} (z-m)}, \quad z = (x, \xi) \in \mathbb{R}^{2n} \quad (4.38)$$

where $c_{\Gamma} = \det(\Gamma)^{-1/2}$.

Gaussian density matrices are parametrized by their means m and their covariance matrices Γ where we have, as usual

$$m = \int_{\mathbb{R}^{2n}} z \rho^{\Gamma, m}(z) dz, \quad \Gamma_{j,k} = \int_{\mathbb{R}^{2n}} z_j z_k \rho^{\Gamma, m}(z) dz.$$

As we have seen in Remark 3.3, some condition is needed on the covariance matrix Γ such that (4.38) defines a density matrix (i.e a non negative operator). This condition is a version of the Heisenberg uncertainty principle (see a proof in the Appendix). Here J is the matrix of the symplectic form on $\mathbb{R}^n \times \mathbb{R}^n$ and $X = (x, \xi) \in \mathbb{R}^{2n}$.

Proposition 4.2 *$\rho^{\Gamma, m}(X)$ defines a density matrix if and only if $\Gamma + i \frac{J}{2} \geq 0$, or equivalently, if and only if the symplectic eigenvalues of Γ are greater than $\frac{1}{2}$.*

Moreover, up to a conjugation by a unitary metaplectic transform in $L^2(\mathbb{R}^n)$, $\rho^{\Gamma, 0}$ is a product of one degree of freedom thermal states \mathcal{T}_{β} (Remark 3.3).

$\rho^{\Gamma, m}(X)$ determines a pure state if and only if 2Γ is positive and symplectic or equivalently $2\Gamma = FF^{\top}$ where F is a linear symplectic transformation.

From these results we can compute the purity (hence the linear entropy) and the von Neumann entropy of Gaussian states.

For the purity we have the straightforward computation:

$$p_{ur}(\hat{\rho}^{\Gamma, m}) = (2\pi)^{-n} \int_{\mathbb{R}^{2d}} \rho^{\Gamma, m}(z)^2 dz = 2^{-n} (\det \Gamma)^{-1/2}. \quad (4.39)$$

Concerning the von Neumann entropy we begin by the computation for thermal states with $n = 1$ and temperature $T = \frac{1}{\beta}$. For simplicity we compute with the Neper logarithm “ln”. We have

$$\hat{\rho}_\tau = Z(\beta)^{-1} e^{-\beta \hat{H}_{osc}}$$

where $\tau = \tanh(\beta/2)$ and $\ln(e^{-\beta \hat{H}_{osc}}) = -\beta \hat{H}_{osc}$. Then we have

$$-\text{tr}(\hat{\rho}_\tau \ln \hat{\rho}_\tau) = \frac{\beta}{Z(\beta)} (\text{tr}(\hat{H}_{osc} e^{-\beta \hat{H}_{osc}}) + \ln(Z(\beta)))$$

Recall that $Z(\beta) = \frac{1}{2 \sinh(\beta/2)}$. So we compute

$$\text{tr}(\hat{H}_{osc} e^{-\beta \hat{H}_{osc}}) = -\frac{\partial}{\partial \beta} \text{tr}(e^{-\beta \hat{H}_{osc}}) = \frac{\cosh \beta}{2(\sinh \beta)^2}$$

and we get

$$S_{BN}(\rho_\tau) = \frac{\beta}{2 \tanh(\beta/2)} + \ln(e^{\beta/2} - e^{-\beta/2}).$$

With the parameter τ we get finally the formula:

$$S_{BN}(\hat{\rho}_\tau) = \frac{1}{\ln 2} \left(\frac{1-\tau}{2\tau} \ln \left(\frac{1+\tau}{1-\tau} \right) - \ln \left(\frac{2\tau}{1+\tau} \right) \right) \quad (4.40)$$

The parameter τ is related with the linear entropy:

$$S_\ell(\hat{\rho}_\tau) = 1 - \frac{Z(2\beta)}{Z(\beta)^2} = 1 - \tau, \quad (4.41)$$

These formulas were obtained in [1].

Let us denote $\mathcal{E}(\tau)$ the r.h.s in (4.40). Using Proposition 4.2 and additivity of the von Neumann entropy, we get the following formula for a general Gaussian state with covariance matrix Γ :

$$S_{BN}(\hat{\rho}^{\Gamma, m}) = \sum_{1 \leq j \leq n} \mathcal{E}(\tau_j) \quad (4.42)$$

where τ_1, \dots, τ_n are the symplectic eigenvalues of $\frac{\Gamma^{-1}}{2}$ (see Appendix for more details).

4.3 Time evolution of reduced mixed states

Here we state and prove the main results of this section. It is convenient to work in the interacting setting. Recall that we have

$$\hat{\rho}_S^{(I)}(t) = U_S^*(t) \hat{\rho}_S(0) U_S(t), \quad (4.43)$$

$$\rho_S^{(I)}(t, z) = \rho_S(t, \Phi_S^t(z)) \quad (4.44)$$

Theorem 4.3 *Let $t_c > 0$ be the largest time t_c such that Ψ_{ii}^t is invertible for every $t \in [0, t_c[$. Assume that the environment density matrix $\hat{\rho}_E$ is a Gaussian with means m_E . Then there exist two time-dependent $2d \times 2d$ matrices $A^{(I)}(t)$, $B^{(I)}(t)$, and a time dependent vector $v^{(I)}(t) \in \mathbb{R}^{2d}$ such that for $t \in [0, t_c[$ the Weyl symbol $\rho_S^{(I)}(t, z)$ of the interacting evolution $\hat{\rho}_S^{(I)}(t)$ of the system (S) satisfies the following master equation (Fokker-Planck type equation):*

$$\begin{aligned} \frac{\partial}{\partial t} \rho_S^{(I)}(t, z) &= (A^{(I)}(t) \nabla_z) \cdot z \rho_S^{(I)}(t, z) + (B^{(I)}(t) \nabla_z) \cdot \nabla_z \rho_S^{(I)}(t, z) \\ &\quad + v^{(I)}(t) \cdot \nabla_z \rho_S^{(I)}(t, z). \end{aligned} \quad (4.45)$$

Moreover we have the following formula to compute $A^{(I)}(t)$, $B^{(I)}(t)$

$$A^{(I)}(t)^\top = -J_S G(t) \Psi_{ei}^t (\Psi_{ii}^t)^{-1} \quad (4.46)$$

$$B^{(I)}(t) = \frac{L(t) + L(t)^\top}{2}, \text{ where} \quad (4.47)$$

$$L(t) = J_S \cdot G(t) (\Psi_{ee}^t - \Psi_{ei}^t (\Psi_{ii}^t)^{-1} \Psi_{ie}^t) \text{Cov}_{\rho_E}(\Psi_{ie}^t)^\top \quad (4.48)$$

$$v^{(I)}(t) = -J_S G(t) \Psi_{ee}^t m_E \quad (4.49)$$

Proof. In this proof (and only here) we shall erase the upper index (I) for the interacting dynamics. Taking the partial trace in the equation (1.3) we have

$$\dot{\rho}_S(t, z) = \int_{\mathbb{R}^{2N}} \{V(t), \rho(t)\}(z, u) du$$

For simplicity we shall assume that $m_E = 0$. It is not difficult to take this term into account. The Poisson bracket is in the variables (z, u) but due to integration in u we have only to consider the Poisson bracket in z . Hence we get

$$\dot{\rho}_S(t, z) = - \int_{\mathbb{R}^{2N}} J_S G(t) u \cdot \nabla_z \rho(t, z, u) du \quad (4.50)$$

where $\rho(t, z, u) = \rho(0, \Psi^{-t}(z, u))$.

Denote by $\tilde{f}(\zeta)$ the Fourier transform of f in the variable z . Then we have

$$\tilde{\rho}_S(t, \zeta) = i\zeta \cdot \int_{\mathbb{R}^{2(d+N)}} J_S G(t) u \rho(0, \Psi^{-t}(z, u)) e^{-iz \cdot \zeta} dz du$$

Now let us perform the symplectic change of variable $(z', u') = \Psi^{-t}(z, u)$. Then we get, using the splitting assumption at $t = 0$,

$$\tilde{\rho}_S(t, \zeta) = i\zeta \cdot \int_{\mathbb{R}^{2(d+N)}} dz' du' J_S G(t) (\Psi_{ei}^t z' + \Psi_{ee}^t u') \rho_S(z') \rho_E(u') e^{-i\zeta \cdot (\Psi_{ii}^t z' + \Psi_{ie}^t u')}. \quad (4.51)$$

Let us denote $\varphi = \Psi_{ii}^t z' + \Psi_{ie}^t u'$ and using the equality

$$i(\Psi_{ii}^t)^{-1} \nabla_\zeta e^{-i\zeta \cdot \varphi} = (z' + (\Psi_{ii}^t)^{-1} \Psi_{ie}^t u') e^{-i\zeta \cdot \varphi}$$

we get

$$\begin{aligned} \tilde{\rho}_S(t, \zeta) &= -\zeta \cdot J_S G(t) \Psi_{ei}^t (\Psi_{ii}^t)^{-1} \nabla_\zeta \tilde{\rho}_S(t, \zeta) \\ &\quad - i\zeta \cdot \int_{\mathbb{R}^{2(d+N)}} dz' du' J_S G(t) \Psi_{ei}^t (\Psi_{ii}^t)^{-1} \Psi_{ie}^t(u') \rho_E(u') \rho_S(z') e^{-i\zeta \cdot \varphi} \\ &\quad + i\zeta \cdot \int_{\mathbb{R}^{2(d+N)}} dz' du' J_S G(t) (\Psi_{ee}^t u') \rho_E(u') \rho_S(z') e^{-i\zeta \cdot \varphi} \end{aligned} \quad (4.52)$$

To absorb the linear terms in u' we use that ρ_E is a Gaussian, $\rho_E = c_\Lambda e^{-1/2 u \cdot \Lambda u}$, where Λ is positive-definite $2N \times 2N$ matrix and c_Λ a normalization constant. So we have $\Lambda^{-1} \nabla_u \rho_E(u) = u \rho_E(u)$, and integrating by parts we have

$$\dot{\tilde{\rho}}_S(t, \zeta) = -\zeta \cdot A^{(I)}(t)^\top \nabla_\zeta \tilde{\rho}_S(t, \zeta) - (\zeta \cdot L(t) \zeta) \tilde{\rho}_S(t, \zeta). \quad (4.53)$$

We get (4.45) by inverse Fourier transform.

□

We can deduce a master equation for the state $\hat{\rho}_S(t)$ of the system (S) :

Corollary 4.4 *With the notations of Theorem 4.3, the reduced density matrix for the system satisfies the following master equation*

$$\begin{aligned} \frac{\partial}{\partial t} \rho_S(t, z) &= \{H_S, \rho_S(t)\}(z) + (A(t) \nabla_z) \cdot z \rho_S(t, z) + (B(t) \nabla_z) \cdot \nabla_z \rho_S(t, z) \\ &\quad + v(t) \cdot \nabla_z \rho_S(t, z), \quad \text{for } t \in [0, t_c]. \end{aligned} \quad (4.54)$$

where $A(t)$, $B(t)$ and $v(t)$ are given by formulas (4.46) with $\Psi^t = \Phi^t$ (replacing the interacting dynamics by the complete dynamics and $G(t)$ by $G(0) = G$).

Proof. Recall that $\rho(t, z) = \rho^{(I)}(t, \Phi_S^{-t}(z))^2$. So the change of variables $z \mapsto \Phi_S^{-t}z$ gives easily the result. \square

Remark 4.5 $\rho_S(t, z)$ is of course well defined for every time $t \in \mathbb{R}$ but the coefficients of the equation master (4.45) may have singularity at $t = t_c$ as we shall see in examples. We shall see below a physical interpretation of t_c .

A consequence is that $\hat{\rho}_S(0) \mapsto \hat{\rho}_S(t)$ is not always a group of operators.

Let us give a lower bound for the critical time $t_c = \inf\{t > 0, \det(\Phi_{ii}^t) = 0\}$.

Denote $\gamma = \|G\|$ (it is a measure of the strength of the interaction) and $f(t) = \|\Phi_S^t\| + \|\Phi_E^t\|$.

Proposition 4.6 *If $\sup_{t \geq 0} f(t) < +\infty$ then there exists $c > 0$ such that $t_c \geq \frac{c}{\gamma}$.*

If there exist $C, \delta > 0$ such that $f(t) \leq Ce^{\delta t}$ for every $t > 0$ then there exists $C_1 \in \mathbb{R}$ such that $t_c \geq \frac{1}{\delta} \log(\frac{1}{\gamma}) + C_1$. The constants c and C_1 are independant of γ .

Proof. It is enough to work in the interaction representation. Using interacting time evolution Ψ^t for the total classical system $(S) \cup (E)$, we get

$$\|\Psi^t - \mathbb{I}\| \leq \gamma \int_0^t f(s) ds + \gamma \int_0^t f(s) \|\Psi^s - \mathbb{I}\| ds$$

Denote $F(t) = \int_0^t f(s) ds$. Using the Gronwall Lemma and integrating by parts we get

$$\|\Psi^t - \mathbb{I}\| \leq \gamma F(t) + \frac{\gamma^3}{6} F(t)^3 e^{\gamma F(t)} \quad (4.55)$$

From the inequality (4.55) we easily get the Proposition. \square

Remark 4.7 *The coefficients of the equation (4.45) are related with the first and second moments of the reduced density matrix $\rho_S(t)$. Let us denote*

$$m_j^{(I)}(t) = \int_{\mathbb{R}^{2d}} z_j \rho^{(I)}(t, z) dz, \quad \mu_{jk}^{(I)}(t) = \int_{\mathbb{R}^{2d}} z_j z_k \rho^{(I)}(t, z) dz.$$

From (4.45) we get

$$\dot{m}^{(I)}(t) = -(A^{(I)}(t)^T m^{(I)}(t)), \quad \text{where } m^{(I)}(t) = (m_1^{(I)}(t), \dots, m_{2d}^{(I)}(t)) \quad (4.56)$$

Computing directly from (4.50) we get

$$\dot{m}_j^{(I)}(t) = - \int_{\mathbb{R}^{2d+N}} z_j J_S G(t) u \cdot \nabla_z \rho(t, z, u) du dz = (J_S G(t) \Psi_{ei}^t m^{(I)}(0))_j. \quad (4.57)$$

So using (4.34) we get

$$m_j^{(I)}(t) = \Psi_{ii}^t m_j^{(I)}(0). \quad (4.58)$$

²If the Hamiltonians are time dependent, we have to replace Φ_S^{-t} by $\Phi_S^{(0,t)}$

From (4.56) and (4.58) we get again (4.46).

Computations of the second moments, using equation (4.45), gives

$$\dot{\mu}^{(I)}(t) = 2B^{(I)}(t) - (A^{(I),T}(t)\mu^{(I)}(t) + \mu^{(I)}(t)A^{(I),T}(t)). \quad (4.59)$$

As above we can also compute directly using (4.50) and (4.34)

$$\dot{\mu}^{(I)}(t) = \Psi_{ii}^t \mu^{(I)}(0) (\dot{\Psi}_{ii}^t)^\top + \Psi_{ie}^t \mu_E(0) (\dot{\Psi}_{ie}^t)^\top. \quad (4.60)$$

Using that $\mu^{(I)}(t)$ is symmetric we get

$$\dot{\mu}^{(I)}(t) = \frac{d}{2dt} \left(\Psi_{ii}^t \mu^{(I)}(0) (\Psi_{ii}^t)^\top + \Psi_{ie}^t \mu_E(0) (\Psi_{ie}^t)^\top \right) \quad (4.61)$$

$$\mu^{(I)}(t) = \frac{1}{2} \left(\Psi_{ii}^t \mu^{(I)}(0) (\Psi_{ii}^t)^\top + \Psi_{ie}^t \mu_E(0) (\Psi_{ie}^t)^\top \right). \quad (4.62)$$

where $\mu_E(0)$ is the second moments matrix of $\rho_E(0)$.

Remark 4.8 We can get again the formula (3.27) from (4.45). We have $\dot{\rho}_S(0) = 0$ and

$$\ddot{\rho}_S(0) = \dot{A}^{(I)}(0) \nabla_z \rho_S \cdot z \rho_S + \dot{B}^{(I)}(0) \nabla_z \rho_S \cdot \nabla_z \rho_S.$$

So we get

$$\dot{A}^{(I)}(0) = -J_S G J_E G^\top, \quad \dot{B}^{(I)}(0) = -J_S G \text{Cov}_{\rho_E} G^\top J_S$$

and

$$\text{tr}_S(\ddot{\rho}_S(0) \hat{\rho}_S(0)) = \frac{1}{2} \text{tr}_{\mathbb{R}^{2d}}(\dot{A}^{(I)}(0)) + (2\pi)^{-d} \int_{\mathbb{R}^{2d}} \dot{B}^{(I)}(0) \nabla_z \rho_S \cdot \nabla_z \rho_S dz,$$

which coincides with formula (3.27) in this particular case.

Remark 4.9 Suppose that the initial state of the total system $(S) \cup (E)$ is Gaussian:

$\rho(0, z, u) = c_\Gamma e^{-(1/2)\Gamma^{-1}(z,u) \cdot (z,u)}$, $c_\Gamma > 0$ is a normalization constant. Then we have the following direct computation for $\rho_S(t, z)$.

We get first the Fourier transform:

$$\tilde{\rho}_S(t, \zeta) = e^{-(1/2)\Gamma(t)(\zeta,0) \cdot (\zeta,0)}$$

where $\Gamma(t) = (\Phi^t) \Gamma (\Phi^t)^\top$. Using inverse Fourier transform we have

$$\rho_S(t, z) = c_{\Gamma,t} e^{-(1/2)\Gamma_S^{-1}(t)z \cdot z} \quad (4.63)$$

where $\Gamma_S(t)$ is the matrix of the positive-definite quadratic form $\zeta \mapsto \Gamma(t)(\zeta, 0) \cdot (\zeta, 0)$ on \mathbb{R}^{2d} and $c_{\Gamma,t} = (2\pi)^{-d} \det^{1/2} \Gamma_t$.

We can see on this example what is the meaning of critical times t_c .

Assume that $\Gamma = \Gamma_S \oplus \Gamma_E$ where $\Gamma_{S,E}$ are positive-definite quadratic forms on \mathbb{R}^{2d} respectively \mathbb{R}^{2N} and let us introduce the following quadratic forms on \mathbb{R}^{2d} .

$$\mathcal{Q}_t(\zeta, \zeta) = \Gamma((\Phi_{ii}^t)^\top \zeta, (\Phi_{ei}^t)^\top \zeta) \cdot ((\Phi_{ii}^t)^\top \zeta, (\Phi_{ei}^t)^\top \zeta)$$

We have $\mathcal{Q}_0(\zeta, \zeta) = \Gamma_S \zeta \cdot \zeta$ and

$$\mathcal{Q}_t(\zeta, \zeta) = \Gamma_S (\Phi_{ii}^t)^\top \zeta \cdot (\Phi_{ii}^t)^\top \zeta + \Gamma_E (\Phi_{ei}^t)^\top \zeta \cdot (\Phi_{ei}^t)^\top \zeta \quad (4.64)$$

We see from (4.64) that the initial state $\hat{\rho}_S(0)$ cannot be recovered from its evolution at time t_c : only the restriction of \mathcal{Q}_0 to $(\ker \Phi_{ii})^\perp$ is recovered from \mathcal{Q}_{t_c} . The physical interpretation is that a part of information contained in $\hat{\rho}_S(t_c)$ has escaped in the environment represented here by Γ_E .

We shall see now that the master equation (4.45) can be easily solved by the characteristics method after a Fourier transform. As in the proof of the Theorem 4.3, $\tilde{\rho}_S^{(I)}(t, \zeta)$ denotes the Fourier transform of $\rho_S^{(I)}(t)$.

Theorem 4.10 *Assume that the means of the environment state is 0. With the notations of the Theorem 4.3 we have:*

$$\tilde{\rho}_S^{(I)}(t, \zeta) = \tilde{\rho}_S(0, (\Psi_{ii}^t)^\top \zeta) \exp \left(-\frac{1}{2} \zeta \cdot \Theta^{(I)}(t) \zeta \right), \quad \forall t \in \mathbb{R}, \quad (4.65)$$

where $\Theta^{(I)}(t) = \Psi_{ie}^t \text{Cov}_{\rho_E(0)}(\Psi_{ie}^t)^\top$.

Remark 4.11 *The interpretation of the r.h.s in formula (4.65) is the following: the first factor is a transport term. The second term is a dissipation term due to the influence of the environment which is controlled by the non negative matrix $\Theta^{(I)}(t)$.*

Formula (4.10) is an extension of a formula obtained in [10] for the Brownian quantum motion model where $\Theta^{(I)}(t)$ is named the "thermal covariance" because the environment is in a thermal equilibrium state.

Proof. In the proof of the Theorem 4.3 we have seen that we have $A^{(I)}(t)^\top = -\dot{\Psi}_{ii}^{(t,0)} \Psi_{ii}^{(0,t)}$.

Here it is convenient to use the notation $\Psi^{(t,s)}$ for the evolution of Ψ^t at time t starting from initial data at time s , as it is usual for non autonomous time dependent evolution equations.

So the characteristic system for the equation (4.53) is the linear differential equation

$$\dot{\zeta} = -(\dot{\Psi}_{ii}^{(t,0)} \Psi_{ii}^{(0,t)})^\top \zeta, \quad \zeta(0) = \zeta_0. \quad (4.66)$$

It is clear that the solution of (4.66) is $\zeta(t) = (\Psi_{ii}^{(0,t)})^\top \zeta_0$. So we have

$$\tilde{\rho}_S^{(I)}(t, \zeta) = \tilde{\rho}_S(0, (\Psi_{ii}^t)^\top \zeta) \exp \left(\int_0^t b(s, \Psi_{ii}^{(s,t)} \zeta) ds \right) \quad (4.67)$$

for $0 \leq s \leq t < t_c$, where $b(s, \zeta) = \zeta \cdot B^{(I)}(s) \zeta$.

But an easy computation shows that we have the following relation

$$B^{(I)}(s) = \frac{1}{2} \left(A^{(I)}(t)^\top \Theta^{(I)}(t) + \Theta^{(I)}(t) A^{(I)}(t) + \frac{d}{dt} \Theta^{(I)}(t) \right).$$

Integrating by parts gives

$$\int_0^t b(s, (\Psi_{ii}^{(t,s)})^\top \zeta) ds = -\frac{1}{2} \zeta \cdot \Theta^{(I)}(t) \zeta$$

and formula (4.65) follows.

□

It is not difficult to go back to the evolution of $\tilde{\rho}_S$ using a change of variable and to the time evolution of $\rho_S(t)$ using inverse Fourier transform.

Corollary 4.12 *Under the conditions of Theorem 4.10 we have the following formula*

$$\tilde{\rho}_S(t, \zeta) = \tilde{\rho}_S(0, (\Phi_{ii}^t)^\top \zeta) \exp \left(-\frac{1}{2} \zeta \cdot \Theta(t) \zeta \right), \quad (4.68)$$

with $\Theta(t) = \Phi_{ie}^t \text{Cov}_{\rho_E}(\Phi_{ie}^t)^\top$.

In particular if $\hat{\rho}(0)$ is a Gaussian state with covariance matrix $\Gamma_S(0)$ then $\hat{\rho}_S(t)$ is a Gaussian state with the following covariance matrix $\Gamma_S(t)$

$$\Gamma_S(t) = \Phi_{ii}^t \Gamma_S(0) (\Phi_{ii}^t)^\top + \Phi_{ie}^t \Gamma_E(0) (\Phi_{ie}^t)^\top, \quad \forall t \in \mathbb{R}, \quad (4.69)$$

where $\Gamma_E(0) = \text{Cov}_{\rho_E}$ is the initial covariance of the environment.

The formula (4.68) is related with Remark 4.7 where we have computed the second moments matrix of $\hat{\rho}_S^{(I)}(t)$.

As far as Φ_{ii}^t is invertible we see from (4.68) that the time evolution of $\hat{\rho}_S$ is reversible but this is no more true for $t \geq t_c$.

From formula (4.68) we get an explicit representation formula for the reduced density of the system as a convolution integral:

Corollary 4.13 *With the notations of Corollary 4.12, we have*

$$\begin{aligned}\rho_S^{(I)}(t, z) &= c_S^{(I)}(t) \int_{\mathbb{R}^{2d}} \rho_S(0, \Psi_{ii}^{(0,t)} z') \exp\left(-\frac{1}{2}(z - z') \cdot \Theta^{(I)}(t)^{-1}(z - z')\right) dz', \\ \rho_S(t, z) &= c_S(t) \int_{\mathbb{R}^{2d}} \rho_S(0, \Phi_{ii}^{(0,t)} z') \exp\left(-\frac{1}{2}(z - z') \cdot \Theta(t)^{-1}(z - z')\right) dz'.\end{aligned}\quad (4.70)$$

where $c_S^{(I)}(t) = (2\pi)^{-d/2} \det(\Psi_{ii}^t)^{-1} \det(\Theta^{(I)})^{-1/2}$ and

$c_S(t) = (2\pi)^{-d/2} \det(\Phi_{ii}^t)^{-1} \det(\Theta)^{-1/2}$.

If $\det(\Phi_{ii}^t) = 0$ or if $\det((\Phi_{ie}^t(\Phi_{ie}^t)^\top)) = 0$, integrals in (4.70) are defined as convolutions of distributions.

Formula (4.70) shows clearly the damping influence of the environment on the system because $\Theta(t)$ is a positive matrix under our assumptions. If $\Theta(t)$ degenerates then the Fourier transform of $\exp(-\frac{1}{2}\zeta \cdot \Theta(t)\zeta)$ is a distribution supported in some linear subspace V_S of \mathbb{R}^{2d} where the damping takes place.

We can deduce an exact formula for the linear entropy $S_\ell(t)$ if $\hat{\rho}_S(0)$ is a Gaussian state.

First, using the Plancherel formula we have

$$\begin{aligned}S_\ell(t) &= 1 - (2\pi)^{-d} \int_{\mathbb{R}^{2d}} (\rho_S(t, z))^2 dz \\ &= 1 - (2\pi)^{-3d} \int_{\mathbb{R}^{2d}} |\tilde{\rho}_S(t, \zeta)|^2 d\zeta\end{aligned}\quad (4.71)$$

$$= 1 - (2\pi)^{-d} \int_{\mathbb{R}^{2d}} \exp(-\zeta \cdot \Theta(t)\zeta) |\tilde{\rho}_S(0, (\Phi_{ii}^t)^\top \zeta)|^2 d\zeta \quad (4.72)$$

If $\rho_S(0)$ is a Gaussian state we have

$$S_\ell(t) = 1 - \det(\Gamma_S(t))^{-1/2} \quad (4.73)$$

where $\Gamma_S(t)$ is given by the formula (4.69).

Remark 4.14 *We have seen in this section that we can compute the quantum evolution of a reduced system when the classical evolution of the blocks Φ_{ii}^t and Φ_{ie}^t of the total system $(S) \cup (E)$ are known. It is hopeless to get general explicit formulas for these blocks, but this is possible in the particular case of two oscillators (Appendix A). For a bath of N oscillators, $1 < N < +\infty$ the problem seems difficult (see Appendix B). For continuous distribution of oscillators many results were obtained concerning the Quantum Brownian Motion model (see references).*

Let us close this section by giving a simple sufficient condition to get correlations between states of the system (S) and the environment (E) . If $\hat{\rho}$ is a state of the total system $(S) \cup (E)$ we say that (S) and (E) are uncorrelated if $\hat{\rho} = \hat{\rho}_S \otimes \hat{\rho}_E$. Note that this decomposition is unique and $\hat{\rho}_{S,E} = \text{tr}_{E,S} \hat{\rho}$. In decoherence theory [8] more difficult notions are also considered: separability and entanglement. $\hat{\rho}$ is separable if there exists a decomposition $\hat{\rho} = \sum_j p_j \hat{\rho}_j^S \otimes \hat{\rho}_j^E$ where $\sum_j p_j = 1$, $p_j \geq 0$, $\hat{\rho}_j^S, \hat{\rho}_j^E$ are pure states respectively in $\mathcal{H}_S, \mathcal{H}_E$. If $\hat{\rho}$ is not separable it is said that $\hat{\rho}$ is entangled.

Proposition 4.15 *Assume that $\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0)$ and that $\hat{\rho}_S(0), \hat{\rho}_E(0)$ are Gaussian states with covariance matrices Γ_S, Γ_E . If the following generic condition is satisfied*

$$J_S \Gamma_S G J_E \Gamma_E^{-1} + G \neq 0 \quad (4.74)$$

then there exists $\varepsilon > 0$ such that for every $t \in]0, \varepsilon]$, $\hat{\rho}(t) \neq \hat{\rho}_S(t) \otimes \hat{\rho}_E(t)$, which means that the reduced system (S) is immediately correlated with its environment (E) when a coupling is switch on.

Proof. The proof is elementary.

We compute with the classical Gaussian state in the interaction representation (as above for simplicity we erase the index (I)). We have

$$\rho(t, z, u) = \rho_S(0, \Psi_{ii}^{(0,t)} z + \Psi_{ie}^{(0,t)} u) \rho_E(0, \Psi_{ee}^{(0,t)} u + \Psi_{ei}^{(0,t)} z).$$

Using the assumptions, we have

$$\rho(t, z, u) = K(t, z) L(t, u) e^{-z \cdot C(t) u} \quad (4.75)$$

where the crossed term is determined by the matrix $C(t)$ satisfying $C(0) = 0$. Using the interacting evolution equation we can easily compute the derivative $\dot{C}(0)$. So we find $\dot{C}(0) = \Gamma_S^{-1} J_S G - G J_E \Gamma_E^{-1}$ and $\dot{C}(0) \neq 0$ if condition (4.74) is satisfied. Hence $C(t) \neq 0$ for t small enough and $t \neq 0$ \square

Remark 4.16 *In [8] the authors have proven a stronger entanglement result for the Quantum Brownian Motion model.*

A Coupled Harmonic oscillators

More explicit computations can be done for systems with two coupled one dimensional harmonic oscillators.

$$\hat{H}_S = \frac{1}{2}(-\partial_x^2 + \omega_S^2 x^2), \quad \hat{H}_E = \frac{1}{2}(-\partial_y^2 + \omega_E^2 y^2).$$

We assume that $\omega_S > 0$ and ω_E can be real positive or purely imaginary ($\omega_E^2 < 0$). $\omega_E^2 > 0$ means a stable environment and $\omega_E^2 < 0$ means an unstable environment. Unstable environment was considered in the paper [4]. Here we revisit the computations of [4].

Let us compute the classical flow of the total Hamiltonian

$$H(x, \xi, y, \eta) = \frac{1}{2}(\xi^2 + \eta^2 + \omega_S^2 x^2 + \omega_E^2 y^2) + \gamma xy.$$

Let $M = \begin{pmatrix} \omega_S^2 & \gamma \\ \gamma & \omega_E^2 \end{pmatrix}$ be the matrix of the quadratic potential for the total system: $V(x, y) = \omega_S^2 x^2 + \omega_E^2 y^2 + \gamma xy$.

The eigenvalues λ_{\pm} of M are

$$\lambda_{\pm} = \frac{1}{2} \left(\omega_S^2 + \omega_E^2 \pm \sqrt{(\omega_S^2 - \omega_E^2)^2 + 4\gamma^2} \right)$$

So we have

$$M = P \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} P^{-1}$$

where $P = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$ and

$$\begin{aligned} \cos \theta &= \left(\frac{1}{2} \left(1 + \frac{\omega_S^2 - \omega_E^2}{(\omega_S^2 - \omega_E^2)^2 + 4\gamma^2} \right)^{1/2} \right) \\ \sin \theta &= \left(\frac{1}{2} \left(1 - \frac{\omega_S^2 - \omega_E^2}{(\omega_S^2 - \omega_E^2)^2 + 4\gamma^2} \right)^{1/2} \right) \end{aligned} \quad (\text{A.76})$$

Now we compute the matrix of Φ^t in the canonical basis of $\mathbb{R}_x \times \mathbb{R}_y \times \mathbb{R}_\xi \times \mathbb{R}_\eta$

$$e_x = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad e_y = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad e_\xi = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_\eta = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

We have $\Phi^t = \Pi \Phi_{\text{diag}}^t \Pi^{-1}$ where

$$\Pi = \begin{pmatrix} P & 0_2 \\ 0_2 & P \end{pmatrix},$$

and

$$\Phi_{\text{diag}}^t = \begin{pmatrix} \cos(t\lambda_+^{1/2}) & 0 & \lambda_+^{-1/2} \sin(t\lambda_+^{1/2}) & 0 \\ 0 & \cos(t\lambda_-^{1/2}) & 0 & \lambda_-^{-1/2} \sin(t\lambda_-^{1/2}) \\ -\lambda_+^{1/2} \sin(t\lambda_+^{1/2}) & 0 & \cos(t\lambda_+^{1/2}) & 0 \\ 0 & -\lambda_-^{1/2} \sin(t\lambda_-^{1/2}) & 0 & \cos(t\lambda_-^{1/2}) \end{pmatrix}$$

The coefficients of the matrix Φ^t are easily computed using the formula

$$e_\alpha \cdot \Phi^t e_\beta = \Pi^{-1} e_\alpha \cdot \Phi_{\text{diag}}^t \Pi^{-1} e_\beta.$$

Let us denote $\Phi^t(j, k)$ the coefficient with row index j and column index k of the matrix Φ^t . This matrix has four 2×2 blocks: $\Phi_{ii}^t, \Phi_{ie}^t, \Phi_{ei}^t, \Phi_{ee}^t$. (16 terms). So we have $\Phi_{ii}^t(j, k) = \Phi^t(j, k)$ for $j, k \in \{1, 2\}$, $\Phi_{ie}^t(j, k) = \Phi^t(j, k)$ with $j \in \{1, 2\}$, $k \in \{3, 4\}$, $\Phi_{ei}^t(j, k) = \Phi^t(j, k)$ with $j \in \{3, 4\}$, $k \in \{1, 2\}$, $\Phi_{ee}^t(j, k) = \Phi^t(j, k)$ with $j, k \in \{3, 4\}$,

$$\Phi_{ii}^t(1, 1) = \cos^2 \theta \cos(t\lambda_+^{1/2}) + \sin^2 \theta \cos(t\lambda_-^{1/2}) \quad (\text{A.77})$$

$$\Phi_{ii}^t(1, 2) = \lambda_+^{-1/2} \cos^2 \theta \sin(t\lambda_+^{1/2}) + \lambda_-^{-1/2} \sin^2 \theta \sin(t\lambda_-^{1/2}) \quad (\text{A.78})$$

$$\Phi_{ii}^t(2, 1) = -\lambda_+^{1/2} \cos^2 \theta \sin(t\lambda_+^{1/2}) - \lambda_-^{1/2} \sin^2 \theta \sin(t\lambda_-^{1/2}) \quad (\text{A.79})$$

$$\Phi_{ii}^t(2, 2) = \cos^2 \theta \cos(t\lambda_+^{1/2}) + \sin^2 \theta \cos(t\lambda_-^{1/2}) \quad (\text{A.80})$$

We have analogous formula for the blocks $\Phi_{ie}^t, \Phi_{ei}^t, \Phi_{ee}^t$.

$$\Phi_{ie}^t(1, 1) = \sin \theta \cos \theta (\cos(t\lambda_+^{1/2}) - \cos(t\lambda_-^{1/2})) \quad (\text{A.81})$$

$$\Phi_{ie}^t(1, 2) = \sin \theta \cos \theta (\lambda_+^{-1/2} \sin(t\lambda_+^{1/2}) - \lambda_-^{-1/2} \sin(t\lambda_-^{1/2})) \quad (\text{A.82})$$

$$\Phi_{ie}^t(2, 1) = \sin \theta \cos \theta (-\lambda_+^{1/2} \sin(t\lambda_+^{1/2}) + \lambda_-^{1/2} \sin(t\lambda_-^{1/2})) \quad (\text{A.83})$$

$$\Phi_{ie}^t(2, 2) = \sin \theta \cos \theta (\cos(t\lambda_+^{1/2}) - \cos(t\lambda_-^{1/2})) \quad (\text{A.84})$$

We note that $\Phi_{ei}^t = \Phi_{ie}^t$.

$$\Phi_{ee}^t(1, 1) = \cos^2 \theta \cos(t\lambda_-^{1/2}) + \sin^2 \theta \cos(t\lambda_+^{1/2}) \quad (\text{A.85})$$

$$\Phi_{ee}^t(1, 2) = \lambda_-^{-1/2} \cos^2 \theta \sin(t\lambda_-^{1/2}) + \lambda_+^{-1/2} \sin^2 \theta \sin(t\lambda_+^{1/2}) \quad (\text{A.86})$$

$$\Phi_{ee}^t(2, 1) = -\lambda_-^{1/2} \cos^2 \theta \sin(t\lambda_-^{1/2}) - \lambda_+^{1/2} \sin^2 \theta \sin(t\lambda_+^{1/2}) \quad (\text{A.87})$$

$$\Phi_{ee}^t(2, 2) = \cos^2 \theta \cos(t\lambda_-^{1/2}) + \sin^2 \theta \cos(t\lambda_+^{1/2}) \quad (\text{A.88})$$

In particular we have

$$\det(\Phi_{ii}^t) = 1 + 2 \sin^2 \theta \cos^2 \theta$$

$$\left(\cos(t\lambda_+^{1/2}) \cos(t\lambda_-^{1/2}) + \frac{\lambda_+ + \lambda_-}{2\sqrt{\lambda_+ \lambda_-}} \sin(t\lambda_+^{1/2}) \sin(t\lambda_-^{1/2}) - 1 \right) \quad (\text{A.89})$$

and

$$\det(\Phi_{ii}^t) = 1 + 2 \frac{\gamma^2}{(\omega_S^2 - \omega_E^2)^2 + 4\gamma^2}$$

$$\left(\cos(t\lambda_+^{1/2}) \cos(t\lambda_-^{1/2}) + \frac{\omega_S^2 + \omega_E^2}{2\sqrt{\omega_S^2 \omega_E^2 - \gamma^2}} \sin(t\lambda_+^{1/2}) \sin(t\lambda_-^{1/2}) - 1 \right) \quad (\text{A.90})$$

From equation (A.90) we can compute the critical time t_c . We see here that we may have t_c finite or infinite, depending on the coupling constant γ and on the sign of ω_E^2 .

1. Assume that $\omega_S^2 \omega_E^2 > \gamma^2$ and $\omega_S^2 \neq \omega_E^2$.

We have $\lambda_+ > \lambda_- > 0$. We see easily that, for some constant C depending only on ω_S, ω_E , we have

$$|\det(\Phi_{ii}^t) - 1| \leq C\gamma, \quad \forall t \in \mathbb{R}$$

Then if $\gamma < \frac{1}{C}$, (Φ_{ii}^t) is invertible for every $t \in \mathbb{R}$.

2. If $\omega_S^2 = \omega_E^2$ and $\omega_S^2 > \gamma^2$ we get from (A.90) that there exists $C > 0$ such that Φ_{ii}^t is invertible for $0 \leq t \leq \frac{C}{\gamma}$.

3. If $\omega_S^2 \omega_E^2 < \gamma^2$ then $\lambda_+ > 0 > \lambda_-$. We can find constants C_1, C_2 such that if $\gamma e^{C_2 t} \leq C_1$ then Φ_{ii}^t is invertible.

B On the quantum Brownian motion model

The quantum brownian motion model was introduced in the paper [12]. The starting point is a one degree of freedom system interacting with a large number N of harmonic oscillators. The total (classical) Hamiltonian is the following

$$H(x, \xi; y, \eta) = \frac{\xi^2}{2m} + V(x) + \sum_{1 \leq j \leq N} \frac{\eta_j^2}{2m_j} + k_j (y_j - x)^2. \quad (\text{B.91})$$

where x, ξ are the coordinates of the system, $y = (y_1, \dots, y_N)$ and $\eta = (\eta_1, \dots, \eta_N)$ are the coordinates for the environment. The environment consists in N harmonic oscillators and the system is connected to each oscillator by a spring with constant $k_j > 0$. This model is a particular case of quadratic systems considered in section 4. if $V(x) = \frac{\omega_S^2}{2} x^2$. The Hamiltonian can be splitted as $H = H_S + H_E + H_I$ where

$$H_S = \frac{\xi^2}{2m} + V(x) + \frac{1}{2} \left(\sum_{1 \leq j \leq N} k_j \right) x^2 \quad (\text{B.92})$$

$$H_E = \frac{1}{2} \left(\sum_{1 \leq j \leq N} \frac{\eta_j^2}{m_j} + k_j y_j^2 \right) \quad (\text{B.93})$$

$$H_I = -2x \left(\sum_{1 \leq j \leq N} k_j y_j \right) \quad (\text{B.94})$$

The classical evolution for the Hamiltonian is not explicitly given for $N > 1$ (we have got explicit formula in Appendix A if $N = 1$). It can be seen that the time evolution of the position x of the

system satisfies the following equation [11], assuming $m_j = 1$ for simplicity:

$$m\ddot{x}(t) + \int_0^t K(t-s)\dot{x}(s)ds + V'(x(t)) + K(t)x(0) = F(t) \quad (\text{B.95})$$

where

$$K(t) = \sum_{1 \leq j \leq N} k_j \cos(\sqrt{k_j}t) \quad (\text{B.96})$$

$$F(t) = \sum_{1 \leq j \leq N} y_j(0) \cos(\sqrt{k_j}t) + \eta_j(0) \sin(\sqrt{k_j}t) \quad (\text{B.97})$$

The difficulty here is that equation (B.95) is not an ODE because of the integral term.

In [12, 11] the authors considered a large N limit, and a continuous distribution of oscillators, such that (B.95) is transformed into a stochastic differential equation where the integral term is replaced by the damping term $\gamma\dot{x}(t)$ where γ is a damping constant (Langevin equation).

C Gaussian density matrices

We shall give here a proof of Proposition 4.2. This is consequence of a particular case of the following Williamson theorem (see [22] and [2] Appendix 6).

Theorem C.1 *Let Γ be a positive non degenerate linear transformation in \mathbb{R}^{2N} . Then there exists a linear symplectic transformation S and positive real numbers $\lambda_1, \dots, \lambda_N$ such that*

$$S^\top \Gamma S e_j = \lambda_j e_j, \text{ and } S^\top \Gamma S e_{j+N} = \lambda_j e_{j+N} \quad (\text{C.98})$$

for $1 \leq j \leq N$, where $\{e_1, \dots, e_N, \dots, e_{2N}\}$ is the canonical basis of \mathbb{R}^{2N} .

in [20] the authors gave a simple proof that we recall here. Recall the following known lemma

Lemma C.2 *Let A be a non degenerate antisymmetric linear mapping in \mathbb{R}^{2N} . Then there exists an orthonormal basis $\{v_1, v_1^*, \dots, v_N, v_N^*\}$ of \mathbb{R}^{2N} and positive real numbers $\{\nu_1, \dots, \nu_N\}$, such that*

$$Av_j = \nu_j v_j^*, \quad Av_j^* = -\nu_j v_j.$$

Proof of Lemma C.2 We proceed by induction on N . This is obvious for $N = 1$.

Assume $N \geq 2$. Let ν_1 be an eigenvalue of the symmetric matrix A^2 , $A^2 v_1 = \nu_1 v_1$, $\|v_1\| = 1$. We can choose a vector v_1^* and $a \in \mathbb{R}$ such that $Av_1 = -av_1^*$ and $\|v_1^*\| = 1$. Then we have easily that $v_1 \cdot v_1^* = 0$ and if P is the plane spanned by $\{v_1, v_1^*\}$ then P and P^\perp are invariant by A . So we can apply the induction assumption to A acting in P^\perp and the Lemma is proved. \square

Proof of Theorem C.1 Consider the antisymmetric matrix $A = \Gamma^{-1/2} J \Gamma^{-1/2}$. Using Lemma C.2 we can find an orthogonal matrix R and a diagonal matrix $\Omega = \text{diag}\{\nu_1, \nu_2, \dots, \nu_N\}$, $\nu_j > 0$, $1 \leq j \leq N$ such that

$$R^\top \Gamma^{-1/2} J \Gamma^{-1/2} R = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}$$

Denote $B = \begin{pmatrix} \Omega^{-1/2} & 0 \\ 0 & \Omega^{-1/2} \end{pmatrix}$ and $S = \Gamma^{-1/2} R B$. We get easily that $S^\top \Gamma S = B^2$ and $S^\top J S = J$ so the proof of the Theorem C.1 follows. \square

The N real numbers λ_j in Theorem C.1 are the symplectic eigenvalues of Γ . Using that $S^\top = -J S^{-1} J$ we see that $J\Gamma$ is diagonalizable with eigenvalues $\{\pm \lambda_j, 1 \leq j \leq N\}$ and that $\{\lambda_1, \dots, \lambda_N\}$ are the eigenvalues (with multiplicities) of $|J\Gamma| = (-J\Gamma^2 J)^{1/2}$.

Proof of Proposition 4.2 We can assume that $m = 0$ and we denote $\rho_\Gamma = \rho^{\Gamma,0}$. We use the symplectic normal form for Γ given by Theorem C.1. Let $\hat{R}(S)$ be the metaplectic unitary operator associated with S (see for example [6]). Hence we have

$$\hat{R}(S)^* \hat{\rho}_\Gamma \hat{R}(S) = \hat{\rho}_{S^\top \Gamma S} = \hat{\rho}_{\tau_1} \otimes \hat{\rho}_{\tau_1} \cdots \otimes \hat{\rho}_{\tau_N},$$

where the τ_j are the symplectic eigenvalues of $\frac{\Gamma^{-1}}{2}$. So $\hat{\rho}_\Gamma$ is a density matrix if and only if we have $0 \leq \tau_j \leq 1$ for $1 \leq j \leq d$ (Remark 3.3). This condition means that the symplectic eigenvalues of 2Γ are greater than 1 or equivalently that $2\Gamma + iJ \geq 0$.

We have already seen that if $\hat{\rho}_\Gamma$ is a pure state then we have $2\Gamma = F^\top F$ with F symplectic. Conversely if $2\Gamma = F^\top F$ then $\hat{\rho}_\Gamma$ is the Wigner function of a squeezed state $\hat{R}(F)\varphi_0$, φ_0 being the standard Gaussian (for details see [6]).

Gaussian states are thermal states for positive non degenerate quadratic Hamiltonians and conversely. This can be proved as follows.

Let $H(u) = \frac{1}{2}u \cdot \Lambda u$ where Λ is a positive non degenerate linear transformation in \mathbb{R}^{2N} . We consider symplectic coordinates for u : $y_j = u \cdot e_j$ and $\eta_j = u \cdot e_{j+N}$, $1 \leq j \leq N$.

Using Theorem C.1 we have $H(u) = H_\Delta(Su)$ where S is a symplectic linear transformation and $H_\Delta(u) = \sum_{1 \leq j \leq N} \lambda_j u_j^2$, $u_j = (x_j, \xi_j) \in \mathbb{R}^2$. Applying the metaplectic transformation we have $\hat{H} = \hat{R}(S)\hat{H}_\Delta\hat{R}(S)^*$ and

$$e^{-\beta\hat{H}} = \hat{R}(S)e^{-\beta\hat{H}_\Delta}\hat{R}(S)^*$$

From the Mehler formula for the harmonic oscillator the Weyl symbol W_Δ of $e^{-\beta\hat{H}_\Delta}$ is

$$W_\Delta(y, \eta) = \prod_{1 \leq j \leq N} \frac{\exp(-\tanh(\beta\lambda_j)(y_j^2 + \eta_j^2))}{\cosh(\beta\lambda_j)}$$

so the Weyl symbol W of $e^{-\beta\hat{H}}$ is given by

$$W(y, \eta) = W_\Delta(S^{-1}(y, \eta)).$$

This proves that $\frac{e^{-\beta\hat{H}}}{\text{tr} e^{-\beta\hat{H}}}$ is a Gaussian state. More explicit results are given in [7, 15].

References

- [1] G.S. Agarwal: *Entropy, the Wigner Distribution Function, and the Approach to Equilibrium of a System of Coupled Harmonic Oscillators* Phys. Rev. A 3, 828 (1971)
- [2] V. Arnold: *Mathematical Methods in Classical Mechanics* Springer, Berlin-Heidelberg (1997)
- [3] H.P. Breuer and F. Petruccione: *The Theory of open quantum systems*, Clarendon Press Oxford (2002).
- [4] R. Blume-Kohout and W.H. Zurek: *Decoherence from chaotic environment: an upside down "oscillator" as a model* Phys. Rev. A 68, 032104 (2003).
- [5] A.O. Caldeira and A.J. Leggett : *Influence of damping on quantum interference: An exactly soluble model* Phys. Rev. , **A31**, p. 1059-1066 (1985)
- [6] M. Combes and D. Robert: *Coherent states and applications in Mathematical Physics*, Springer-Verlag (2012).
- [7] I. Dereziński: *Some remarks on Weyl pseudodifferential operators*. Journées EDP, Saint Jean de Monts, expoé XII, 1-14 (1993).

- [8] J. Eisert and M. B. Plenio: *Quantum and Classical Correlations in Quantum Brownian Motion* Phys. Rev. Letters, Vol.89, No.13, 137902, p. 1-4 (2002)
- [9] R. P. Feynman and F.L. Vernon: *The theory of a general quantum system interacting with a linear dissipative system*, Annals of physics, **24** p. 118-173 (1963).
- [10] C. H. Fleming, B. L. Hu and A. Roura: *Exact analytical solutions to the master equation of Brownian motion for a general environment* arXiv:1004.1603v2[quant-ph] (2010) and Ann. Phys. Vol.326, Issue 5, p.1207-1258 (2011)
- [11] G.W. Ford and M. Kac: *On the Quantum Langevin Equation* Journal of Statistical Physics, Vol. 46, Nos. 5/6, (1987)
- [12] G.W. Ford, M. Kac and P.Mazur: *Statistical Mechanics of Assemblies of Coupled Oscillators* J. Math. Phys. **6** p.504-515 (1965)
- [13] G.W. Ford and R.F. O'Connell: *Exact solution of the Hu-Paz-Zhang master equation* Phys. Rev. D, Vol. 64, 105020 1-13 (2001)
- [14] J.J. Halliwell and T. Yu: *Alternative derivation of the Hu-Paz-Zhang master equation of quantum Brownian motion* Phys. Rev. D **53**, p.2012-2019 (1996)
- [15] L. Hörmander: *Symplectic classification of quadratic forms, and general Mehler formulas* Math. Z, 219, 413-449 (1995)
- [16] B.L. Hu, J.P. Paz and Y. Zhang: *Quantum Brownian motion in a general environment: Exact master equation with nonlocal dissipation and colored noise* Phys. Rev. D **45**, p.2843-2861 (1992)
- [17] K. Hornberger: *Introduction to Decoherence, Entanglement and Decoherence* Lecture Notes in Physics, Vol. 768 p. 221-276 (2009)
- [18] M.A. Nielsen and I.L. Chuang: *Quantum computation and quantum information*, Cambridge University Press (2000).
- [19] M. Schlosshauer: *Decoherence and the quantum-to-classical transition*, Springer-Verlag (2007).
- [20] R. Simon, S. Chaturvedi and V. Srinivasan: *Congruences and canonical forms for a positive matrix: application to Schweinler-Wigner extremum principle* J. Math. Phys. 40, p.3632-3643 (1999)
- [21] R. Simon, E.C.G. Susarshan and N. Mukada: *Gaussian Wigner distributions : a complete characterization* Phys. Rev. **A 36** p. 3868-3873, (1987)
- [22] J. Williamson: *On algebraic problem concerning the normal forms of linear dynamical systems* Amer. J. of Math. **58**, N.1, p.141-163, (1936)